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High Production Volume (HPV) Chemical Challenge Program

TEST PLAN

For The

Fuel Oils Category

Prepared by:

American Chemistry Council
Olefins Panel
HPV Implementation Task Group

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PLAIN ENGLISH SUMMARY

This test plan addresses streams that are products of the ethylene process and are used as fuel oils. The Fuel Oils Category includes CAS numbers that represent streams with a carbon number distribution that ranges predominantly from C8 and higher. The plan addresses the category by evaluating the data available for representative streams, as well as for chemicals and products not in this category whose data can be used to read across to products in this category. Supporting data on key chemical components, such as naphthalene and biphenyl, will be reviewed as part of other test plans under the EPA High Production Volume (HPV) Challenge Program, the ICCA (International Council of Chemical Associations) program, or from chemicals already sponsored in the European Union Existing Substances Risk Assessment program or the OECD (Organization for Economic Cooperation and Development) SIDS (Screening Information Data Sets) program. No additional toxicity testing for potential human health effects is necessary. However, aquatic toxicity and biodegradation tests will be conducted to fully characterize these streams. In addition, data and/or technical discussions will be prepared for the remaining fate endpoints, and a comprehensive physicochemical database will be developed that contains measured and calculated data.

EXECUTIVE SUMMARY

The Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies hereby submit for review and public comment the Fuel Oils Category test plan under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. It is the intent of the Panel and its member companies to use new information in conjunction with a variety of existing data and scientific judgment/analysis to adequately characterize the SIDS (Screening Information Data Set) human health, environmental fate and effects, and physicochemical endpoints for this category.

This test plan addresses streams that are products of the ethylene process that contain mostly cyclic olefins and aromatic hydrocarbons that are generally carbon number 8 and higher, with some lighter components. The streams are similar in that they are all complex streams (containing several different chemicals) that generally consist of the same higher-boiling hydrocarbons, but at varying concentrations. These streams are represented using 12 CAS numbers. The streams are frequently utilized in the fuel oil market and sometimes for chemical purposes. This test plan addresses the category by evaluating data on select mixed process streams that represent typical fuel oil products. Robust summaries are provided for the following:

- Light Pyrolysis Fuel Oil
- Aromatic Pyrolysis Oil and Rerun Tower Bottoms
- Biphenyl Feedstock
- Coal Derived Fuel Oils

Results from studies on these streams will be used to read across to evaluate other members of the Fuel Oils Category. Additional supporting data exist, or will be collected on many of the components of the streams in this category as part of other test plans under the HPV program, the ICCA (International Council of Chemical Associations) program, or from chemicals already sponsored in the OECD (Organization for Economic Cooperation and Development) SIDS (Screening Information Data Sets) program or European Union Existing Substances Risk Assessment program.

Predictive computer models will be used to develop relevant environmental fate and physicochemical data for chemicals in products of the Fuel Oils Category. Environmental fate information will be summarized either through the use of computer models when meaningful projections can be developed or in technical discussions when computer modeling is not applicable. For mixed streams, physicochemical properties will be represented as a range of values according to component composition. These data will be calculated using a computer model cited in an EPA guidance document prepared for the HPV Challenge Program.

In preparing this test plan, the Panel has given careful consideration to the principles contained in the letter EPA sent to all HPV Challenge Program participants on October 14,

1999. As directed by EPA in that letter, the Panel has sought to maximize the use of scientifically appropriate categories of related chemicals and structure activity relationships. Additionally, and also as directed in EPA's letter, in analyzing the adequacy of existing data, the Panel has conducted a thoughtful, qualitative analysis rather than a rote checklist approach. The Panel has taken the same thoughtful approach when developing its test plan. The Panel believes its test plan conforms to the principles articulated in EPA's letter.

After careful evaluation of the existing data, no additional toxicity testing for potential human health effects is proposed. However, aquatic toxicity and biodegradation tests are proposed to characterize the potential toxicity of these streams to the environment within the HPV program. In addition, data and/or technical discussions will be prepared for the remaining fate endpoints, and a comprehensive physicochemical database will be developed that contains measured and calculated data.

LIST OF MEMBER COMPANIES
THE OLEFINS PANEL

The Olefins Panel includes the following member companies:

ATOFINA Petrochemicals, Inc.*
BP Chemical Company*
Chevron Phillips Chemical Company LP
The Dow Chemical Company
E.I.du Pont de Nemours and Company*
Eastman Chemical Company
Equistar Chemicals, LP
ExxonMobil Chemical Company
Formosa Plastics Corporation, U.S.A.
The Goodyear Tire & Rubber Company*
Huntsman Corporation
Koch Industries*
NOVA Chemicals Inc.*
Noveon, Inc.*
Sasol America, Inc.*
Shell Chemical Company*
Sunoco, Inc.*
Texas Petrochemicals Corporation*
Westlake Chemical Corporation*
Williams Olefins, LLC*

*These companies are part of the Olefins Panel but do not produce streams in the Fuel Oils Category

TABLE OF CONTENTS
TEST PLAN FOR THE FUEL OILS CATEGORY

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I. INTRODUCTION

The Olefins Panel (Panel) of the American Chemistry Council and the Panel's member companies have committed to develop screening level human health effects, environmental effects and fate, and physicochemical data for the Fuel Oils Category under the Environmental Protection Agency's (EPA's) High Production Volume (HPV) Challenge Program (Program).

In preparing this test plan, the Panel has given careful consideration to the principles contained in the letter EPA sent to all HPV Challenge Program participants on October 14, 1999. As requested by EPA in that letter, the Panel has sought to maximize the use of scientifically appropriate categories of related chemicals and of structure activity relationships. The Panel has coordinated with other industry groups covering related chemicals. Additionally, and also as requested in EPA's letter, in analyzing the adequacy of existing data, the Panel has conducted a thoughtful, qualitative analysis rather than a rote checklist approach. The Panel has taken the same thoughtful approach when developing this revised test plan and believes it conforms to those principles.

This plan identifies CAS numbers used to describe process streams in the category, identifies existing data of adequate quality for products included in the category, and outlines testing needed to develop screening level data for this category under the Program. This document also provides the testing rationale for the Fuel Oils Category. The objective of this effort is to identify and develop sufficient test data and/or other information to characterize the human and environmental health and environmental fate for the category in compliance with the EPA HPV Program. Physicochemical data that are requested in this program will be developed and calculated as described in the EPA guidance documents.

II. DESCRIPTION FOR THE FUEL OILS CATEGORY

A. The Category

The Fuel Oils Category was developed by grouping 8 ethylene industry streams made up of hydrocarbons that are generally carbon number 8 (i.e. C8) and higher with varying amounts of lower boiling materials. The streams are similar in that they are all complex streams that consist predominantly of the same higher-boiling hydrocarbons, mostly cyclic olefins and aromatics, but at varying concentrations. The Panel believes these streams are similar from both a process and a toxicology perspective, which is why this group is considered a category for purposes of the HPV Program. Twelve CAS numbers (Table 1) are used to describe the 8 process streams (Table 2) arising from the ethylene process that are commercial products or isolated intermediates. A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The CAS numbers used to represent these mixed streams are generally vague with respect to the specifics that distinguish the streams within

the category. Therefore, more than one CAS number may correctly represent a single stream and a CAS number may be applicable to more than one stream. A description of the ethylene and associated stream production processes is included in Appendix 1.

The streams in this category consist of complex hydrocarbon reaction products with a carbon number distribution that is predominantly in a C8 and higher range. The 1,3-butadiene content is negligible. The typical compositions of the streams in this category are shown in Table 3. Descriptions of the eight streams in the Fuel Oils Category are presented below.

B. Fuel Oils Streams

(1) Heavy Pyrolysis Fuel Oil from the Ethylene Process Unit: In ethylene plants cracking liquid feedstocks, the cracking furnace effluent (after heat recovery) is further quenched by injection of recycled quench oil. This step results in the condensation of higher boiling hydrocarbon compounds that are typically separated from the rest of the furnace effluent as the bottoms of the primary fractionation tower or oil quench tower. Lights are stripped from the excess oils generated from this quench system, resulting in the stream identified here as heavy pyrolysis fuel oil consisting of C10+ and considerable PAHs.

(2) Light Pyrolysis Fuel Oil from the Ethylene Process Unit: In some cases, a light pyrolysis fuel oil is produced from the oil quench system in an ethylene plant that cracks liquid feedstocks. This stream may be produced as a side draw from the primary fractionation tower. The stream typically has a carbon number distribution of C9 to C14 and the major components are naphthalene (30 to 60%), methyl naphthalenes and other substituted one and two ring aromatics.

(3) Quench Oil from the Ethylene Process Unit Water Quench System: In ethylene plants cracking only gases, the cracking furnace effluent (after heat recover) may be further quenched with water. This step results in the condensation of a relatively small amount of higher boiling hydrocarbon components that, after stripping to remove lights, may be isolated as the Quench Oils from of the Ethylene Process Unit water quench system. This stream is predominant C7 through components boiling at 650°F or higher. The reported composition indicates 0.1 % benzene, 5% toluene, 12% C8 aromatics, 5% naphthalene, 10% anthracene and 65% C7-C18 cyclic olefins.

(4) Pyrolysis Fuel Oil from Pyrolysis Gasoline Distillation: This stream is separated by distillation from pyrolysis gasoline, as a bottoms product. The reported composition indicates a carbon number distribution of from C9 to hydrocarbons boiling at 650°F or higher. The reported typical composition includes 20% dicyclopentadiene, 30% codimers of C5 and C6 monomers, 20% naphthalene and substituted naphthalenes.

(5) Combined Fuel Oil of the Ethylene Process and Pyrolysis Gasoline Units: A single combined fuel oil stream for the ethylene process unit and the pyrolysis gasoline unit is not an uncommon situation for the industry. The carbon number distribution for this stream is generally C10 to compounds with a boiling point of 650°F or higher. At least in some cases, lower carbon number components are reported for the stream, e.g. C5s at approximately 2%

and benzene at up to 4%. The major components reported in the stream are typically 25% C9 compounds, 10-47% naphthalene and 4-30% methylnaphthalenes.

(6) Combined Fuel Oil from Benzene Hydrodealkylation (HDA) and Pyrolysis Fuel Oils: Ethylene process operations that include both a pyrolysis gasoline distillation unit and a benzene hydrodealkylation unit may combine the fuel oil streams from these two units resulting in a single isolated product. Fuel oil is produced in the benzene HDA process by the HDA reactors and separated as a distillation bottoms product. The carbon number distribution for this combined fuel stream is C9 through hydrocarbons with a boiling point of 650°F or higher, although relatively low levels of lower carbon number hydrocarbons may be present, e.g. 0.2% benzene. The major components reported in the stream include 11% C9 aromatics to naphthalene, 7.5-12% DCPD, 7-13% naphthalene, 22% methylnaphthalenes, and 25-35% biphenyl.

(7) Hydrotreated Flux Oil: This is a hydrotreated fuel oil stream with a carbon number distribution predominantly C10 to hydrocarbons with a boiling point of 650°F or higher. The stream may be produced as distillation bottoms from a pyrolysis gasoline hydrotreator unit. The components in the stream are predominantly aromatics, paraffins and cyclic compounds. This stream differs from the other fuel oils describe above in that its diolefin and vinyl aromatic content is very low.

(8) Biphenyl Concentrate: Biphenyl concentrate is a coproduct of the benzene hydrodealkylation unit that is isolated by distillation from the HDA reactor effluent. The carbon number distribution for the stream is C7 to C18, with the major component reported to be 65 to 95% biphenyl.

III. TEST PLAN RATIONALE

A. Mammalian/Human Health Effects and Test Strategy

The Fuel Oils Category consists of mixed hydrocarbon streams with a carbon number distribution that is predominantly C8 and higher. The toxic effects are dependent on the chemical composition and can be discussed as those attributed to the ≤C9 fraction, the C10 to C12 fraction, and the >C12 components. A number of the components of the streams listed in this category (see Table 3) are already SIDS (Screening Information Data Set) listed materials. Some of the remaining components will be tested as part of other test categories or by other groups within the HPV or ICCA programs. The toxicity of the ≤C9 components is similar to the hydrocarbon solvent materials being covered under the International Hydrocarbon Solvents Consortium HPV Program, and will not be further discussed in this test plan. Two of the C10-C12 materials are SIDS chemicals, naphthalene and dicyclopentadiene, and the C12 biphenyl has been volunteered for the HPV Challenge program by SOCMA (Synthetic Organic Chemical Manufacturers Association). Additionally, several component materials are undergoing risk assessment in Europe (i.e., toluene and naphthalene). Because biphenyl may be present in the Fuel Oils at

concentrations up to 95%, naphthalene at >50%, and DCPD up to 20%, the toxicity of these component materials is summarized below.

Biphenyl

The health hazards of biphenyl have been reviewed (EPA, 1984). Biphenyl is not particularly toxic by ingestion; the oral LD_{50} for the rat is 3280 mg/kg (Deichmann *et al.*, 1947), 1900 mg/kg for the mouse (Isshiki *et al.*, 1983), and for the rabbit, it is 2400 mg/kg. (Deichmann *et al.*, 1947) Intradermal injections in guinea pigs produced local necrosis and some evidence of an allergenic response. (Haley *et al.*, 1959) Repeated application of a 25% solution in olive oil to rabbit skin at 0.5 g/kg/day, 5 days/week, caused no local irritation, but these treatments did result in the death of one rabbit after 8 applications and weight loss in three others after 20 applications. (Deichmann *et al.*, 1947)

Repeated inhalation exposure by rats of biphenyl dust, impregnated on diatomaceous earth, caused irritation of the nasal mucosa, labored breathing with bronchopulmonary lesions, and slight toxic effects on liver and kidneys at a concentration of 300 mg/m^3, 7 hours/day for 64 days. Five rats died between the 29th and 49th exposure days. Rabbits were unaffected, but mice exposed at 5 mg/m^3 for this period showed signs of respiratory difficulty. Rats at this concentration were not affected. (Deichmann *et al.*, 1947)

Bionetics Research Labs (BRL, 1968) treated B6AKF1 and B6C3F1 mice (18/sex/strain) with daily gavage doses of 215 mg/kg 1,1- biphenyl in gelatin from days 7 to 28 of age. The mice were then given a diet containing 517 ppm 1,1-biphenyl for the subsequent 18 months. Positive, negative and vehicle controls were included in the study. The animals were weighed every 6 months and histopathologic examination of the lymphatic and pulmonary systems, liver, skin, mammary glands and uterus were performed at the end of the study. No increase in the incidence of tumors was found in any treated group compared with negative and vehicle controls.

Ambrose et al. (1960) fed 15 weanling albino rats/sex/group diets containing 0, 0.001, 0.005, 0.01, 0.05, 0.1, 0.5, or 1% (0, 0.5, 2.5, 5.0, 25, 50, 250, or 500 mg/kg/day) 1,1-biphenyl for 700 days. At the end of the treatment period, histopathologic examination of the mammary gland, pituitary, adrenals, uterus, lungs, bladder, and other tissues was performed. All rats in the 250 and 500 mg/kg/day groups showed evidence of kidney damage, including irregular scarring, lymphocytic infiltration, tubular atrophy and patchy tubular dilation. Decreased food intake, retarded growth and reduced hemoglobin levels were also observed in these groups. Survival appeared reduced in males receiving 250 mg/kg/day and in both sexes at 500 mg/kg/day, although a statistical analysis of survival was not performed. Based on these data it appears that an MTD was achieved. Although not designed as an oncology study, several malignant and benign tumors were found in both the treated and control rats. These were not considered to be related to 1,1- biphenyl treatment. A supporting unpublished study by Stanford Research Institute (SRI, 1960) was cited in which a NOAEL of 0.1% biphenyl in the diet was found in both a subchronic rat feeding study and a three- generation rat reproduction study. A NOAEL of 0.1% of diet is chosen because of the uncertainty of the significance of the effects observed at lower doses as compared to the more certain AEL of

0.5% of diet. The observation of the same NOAEL in a supporting study is also a contributing factor.

SRI (1953) fed diets containing corn oil and 0, 0.01, 0.1, or 1.0% 1,1-biphenyl to groups of 12 male and 12 female Sprague- Dawley rats for 2 years. Malignancies were reported in two rats; one (sex not specified) on the 0.1% diet had an adenocarcinoma of the colon and one female on the 1.0% diet had a peritoneal tumor. Many of the treated and control male rats had tubular dilation of the kidneys to varying degrees of severity; however, the incidence and severity of the renal lesions were greater in the group fed 1.0% 1,1-biphenyl than in the controls. This study is limited by small group sizes, excess mortality due to a refractory fulminating respiratory infection, and concurrent antibiotic therapy.

BRL (1968) treated B6AKF1 and B6C3F1 28-day-old mice (18/sex/strain) with a single subcutaneous 46.4 mg/kg dose of 1,1-biphenyl in DMSO. The mice were observed for 18 months before sacrifice. Gross and microscopic observations were performed on internal body organs of the chest and abdomen. No increase in the incidence of tumors was found in any treated group compared with controls.

Kurata et al. (1986) provided groups of 25 male F344 rats with 0.05% N- butyl-N-(4-hydroxybutyl)nitrosamine (BBN) in the drinking water for 4 weeks followed by either a basal diet or diet containing 0.5% 1,1-biphenyl for 32 weeks. A group of five rats received the 1,1-biphenyl-containing diet without pretreatment with BBN. Rats receiving the 1,1-biphenyl diet, both with and without BBN pretreatment, gained less weight than control rats that received only BBN. In the 18 surviving rats treated with BBN followed by 1,1-biphenyl, the incidences of hyperplasia, papillomas and carcinomas in the urinary bladder was 94, 83 and 61%, respectively. These increases were statistically significant. The incidences of hyperplasia, papillomas and carcinomas in rats treated with BBN alone were 25, 12 and 0%, respectively. Hyperplasia, papillomas and carcinomas were not observed in the 5 rats fed the 1,1- biphenyl-containing diet without pretreatment with BBN. Urinary bladder stones occurred in 25% of rats receiving BBN and 1,1-biphenyl but in only 12% of the BBN control. 1,1-Biphenyl appeared to be a tumor promoter in this experiment.

A modification of the alkaline single cell gel electrophoresis (SCG) (Comet) assay was used to test the *in vivo* genotoxicity of biphenyl in mouse stomach, liver, kidney, bladder, lung, brain, and bone marrow. CD-1 male mice were sacrificed 3, 8, and 24 h after oral administration of 2000 mg/kg biphenyl. DNA damage was induced in all the organs studied, and biphenyl-induced increased DNA migration peaked at 24 h. (Sasaki *et al.*, 1997) The possible genotoxic and teratogenic actions of biphenyl (diphenyl) was investigated in two microbial systems and a metazoan model were used: diploid D7 strain of Saccharomyces cerevisiae; Salmonella typhimurium strains TA100, TA98, TA1535, TA1537, TA1538, TA1532, TA2636; and sea urchins (Paracentrotus lividus and Sphearechinus granularis). Severe toxicity resulted in all of the test organisms at levels greater than or equal to 10(-5) M (approximately 2 ppm). Biphenyl caused genetic effects in yeast with and without activating system. Biphenyl action on sea urchins resulted in developmental defects and mitotic abnormalities, following exposure of embryos or by pretreatment of sperm or eggs. The

minimal active concentration was 10-4 M (Pagano *et al.*, 1983). Biphenyl was not teratogenic in the rat (Khera et al, 1979).

1,1-Biphenyl was not mutagenic in reverse mutation tests in Salmonella and Eshcerichia coli and in a DNA repair test in E. coli (Anderson and Styles, 1978; Cline and McMahon, 1977; Hirayama et al., 1981). 1,1-Biphenyl did not induce chromosomal aberrations in Chinese hamster cells or unscheduled DNA synthesis in rat hepatocytes (Abe and Sasaki, 1977; Ishidate and Odashima, 1977; Brouns et al., 1979). 1,1-Biphenyl did induce forward mutation in mouse lymphoma cells and sister chromatid exchanges in Chinese hamster cells, although a dose-response relationship was not observed in the latter test (Wangenheim and Bolcsfoldi, 1988; Abe and Sasaki, 1977).

Naphthalene

The health hazards of naphthalene have been extensively studied. Recent reviews (European Union 2001, ATSDR 1996) indicate the most sensitive health effect endpoints are hemolytic anemia (humans) and respiratory effects including cancer (rodents). The naphthalene data are extensively discussed in the European Union (EU) Risk Assessment Document for Naphthalene (European Union 2001) and are summarized below.

An oral LD50 value for naphthalene in rats of approximately 1.8 g/kg has been reported. An oral dose of 1.0 g/kg for 2 days produced only slight eye effects in albino rats, whereas rabbits given 2000 mg/kg/day orally for 5 days developed cataracts; even after one or two oral doses of naphthalene at 1000 mg/kg, cataract formation had begun. Rabbits fed repeated doses of 1 g naphthalene/kg/day for up to 20 days showed browning of the lenses and eye humors, degeneration of the retina, and cataract formation.

Mice were exposed to an atmosphere containing 30 ppm naphthalene 6 hours/day for 6 months. This exposure did not elicit a significant increase in lung adenomas; however, an increased incidence of multiple pulmonary alveolar adenomas was observed upon histopathological examination. (Adkins *et al.*, 1986)

In a 2-year inhalation study, groups of male and female mice were exposed at 0, 10, or 30 ppm naphthalene, 6 hours/day, 5 days/week for 103 weeks.(National Toxicology Program 1992) In male mice, there was no increase in the incidence of tumors related to naphthalene exposure. In the female mice, the incidence of pulmonary alveolar/bronchiolar adenomas in the 30 ppm group (28/134, 21%) was significantly increased compared with controls (5/68, 7%). In the nose of both sexes, naphthalene was associated with an increase in the incidence and severity of minimal to mild chronic inflammation, metaplasia of the olfactory epithelium, and hyperplasia of respiratory epithelium. In the lung of both sexes, naphthalene exposure was associated with chronic inflammation. The U.S. National Toxicology Program (NTP) concluded that there was no evidence for the carcinogenicity of naphthalene in male mice and that there was some evidence of carcinogenic activity in female mice (National Toxicology Program 1992).

Groups of male and female rats were exposed by inhalation to 0, 10, 30, or 60 ppm naphthalene, 6 hours/day, 5 days/week for 105weeks. (National Toxicology Program 2000) The incidences of neuroblastoma of the olfactory epithelium, a rare neoplasm, occurred with positive trends in males and females and was considered to be related to naphthalene exposure. In males, the incidence of adenoma of the respiratory epithelium of the nose, another rare neoplasm, occurred with a positive trend and was significantly increased in all exposed groups; none occurred in chamber controls. In females, this neoplasm occurred in the 30 and 60 ppm groups. Because these neoplasms did not occur in the chamber controls they were considered to be related to naphthalene exposure. Increased incidences of nonneoplastic lesions of the nose included atypical hyperplasia, atrophy, chronic inflammation and hyaline degeneration of the olfactory epithelium; hyperplasia, squamous metaplasia, hyaline degeneration, and goblet cell hyperplasia of the respiratory epithelium; and glandular hyperplasia and squamous metaplasia. The NTP concluded that there was clear evidence of carcinogenic activity in male and female rats based on increased incidences of respiratory epithelial adenoma and olfactory epithelial neuroblastoma of the nose (National Toxicology Program 2000).

No studies investigating effects on fertility are available. However, in a carcinogenicity study mice showed no histopathological changes in the epididymis, prostate, seminal vesicle, testis or ovary following inhalation of 30 ppm naphthalene vapor for 6 hours/day, 5 days/week for 104 weeks (estimated to be approximately 45 mg/kg/day) (National Toxicology Program 1992). Similarly, when male mice were given 133 mg/kg/day or 267 mg/kg/day for 90 days, no adverse effects on the testes could be discerned. (Shopp *et al.*, 1984)

In a well-reported developmental toxicity study groups of 25 rabbits were treated by gavage with 0, 20, 80 or 120 mg/kg/day of naphthalene on days 6-19 of gestation (Navarro *et al.*, 1992). Caesarean sections were conducted on day 30. There were no signs of maternal toxicity in any of the treatment groups and there were no differences in the number of resorptions, live and dead fetuses, litter size, fetal body weight and no increase in the incidence of external, skeletal or visceral malformations. The potential to produce developmental effects at maternally toxic doses was not assessed. The dose levels used were based on a preliminary study (which was cited in the above report) in which rabbits were treated with 0, 75, 150, 300 or 500 mg/kg/day, presumably according to the above protocol. Maternal deaths (at least 40%) occurred with 150 mg/kg/day and above. There were no signs of fetotoxicity. Pups were apparently not assessed for malformations. It is difficult to draw firm conclusions from the brief report of this preliminary study that did not assess occurrence of malformations.

In a well conducted unpublished study, groups of 18 rabbits were administered 0, 40, 200 or 400 mg/kg/day naphthalene by gavage on days 6-18 of gestation (Pharmakon, 1985). Caesarean sections were conducted on day 29. Two high dose animals aborted on days 18 and 23 of gestation, which was considered to be due to maternal toxicity. There were no naphthalene induced maternal deaths or statistically significant changes in maternal body weight. However, at 200 and 400 mg/kg/day increased dyspnoea, cyanosis and salivation were reported. Examination of the dams and offspring indicated no differences in the

number of implantations, post-implantation loss, number of live and dead fetuses, litter size, fetal body weight, or fetal sex distribution in any of the treatment groups. Overall, no developmental effects were observed at a naphthalene dose of up to 400 mg/kg/day, at which maternal toxicity was evident.

In a well conducted but poorly reported study groups of 25 female Sprague-Dawley rats were treated by gavage with 0, 50, 150 or 450 mg/kg/day naphthalene on days 6-15 of gestation (Navarro *et al*., 1991). Caesarean sections were performed on day 20. Maternal body weight gains (corrected for gravid uterine weight) were decreased by 22 and 29% with 150 and 450 mg/kg/day respectively. These animals were also lethargic and showed slow respiration rates during the treatment period. There were no differences in the number of corpora lutea per dam or the number of dead or live fetuses per litter in any treatment group. However there was a 2-fold increase in the number of resorptions per litter with the top dose compared to the controls. It was not stated whether these were considered to be early or late resorptions. Pups from top dose animals showed a slight increase in the number of litters with visceral malformations and slight dose-related increases in percentage of fetuses per litter with visceral malformations was also noted. However these increases, which were principally due to increased incidence of enlarged lateral ventricles in the brain, were not statistically significant. Overall this study provides some evidence of fetotoxicity occurring at maternally toxic doses with no fetotoxicity occurring at doses which were not maternally toxic. The dose levels used were based on a preliminary study (cited in the above report) in which rats were treated with 0, 100, 400, 500, 600 or 800 mg/kg/day, presumably according to the protocol above. Severe maternal toxicity was noted with the top two doses. With the top dose 67% of dams died and total resorptions occurred in 33% of the survivors. No further details were presented of the toxicity seen with 600 mg/kg/day. "Slight" maternal and fetal toxicity was noted with 400 and 500 mg/kg/day although no details were given. Pups were not assessed for malformations. Overall fetal toxicity was apparently observed at maternally toxic doses. However it is difficult to draw firm conclusions from the brief report of this preliminary study which did not assess the occurrence of malformations.

In a poorly conducted study in CD-1 mice, groups of 50 females were treated by gavage with 0 or 300 mg/kg/day naphthalene on days 7-14 of gestation (Plasterer *et al*, 1985). Dams showed a 15% decrease in survival and a 26% reduction in body weight. There was a statistically significant decrease (18%) in the number of live pups/litter, although a corresponding increase in the number of dead pups/litter was not noted. There was no change in pup weight. Gross examinations were apparently performed on the pups but it is not clear if visceral and skeletal examinations were conducted. The number of resorptions was not assessed. Overall, evidence of fetal toxicity was observed in this limited study at a dose producing severe maternal toxicity.

Naphthalene was not mutagenic in Salmonella typhimurium (strains TA98, TA100, TA1535, TA1537, (Kraemer *et al.*, 1947; McCann *et al.*, 1975) UTH 8414, or UTH 8413 (18)) either in the presence or absence of a hamster or rat liver (S9) metabolizing system. No evidence for naphthalene mutagenesis was obtained in studies with cultured embryonic rodent (Rhim, 1974; Freeman, 1973) or mammary gland (Tonelli, 1979) cells.

Dicyclopentadiene

DCPD is a mid-range (C10) dicyclic alkene found at varying levels in many of the category streams. DCPD is an OECD SIDS chemical with an established screening data set and hazard profile for human health and environmental effects (OECD, 1998). The toxicology of DCPD has been reviewed by Cavender (1994a) and ECETOC (1991) and a summary of this information follows. Details of key studies pertinent to the OECD SIDS health effects endpoints are provided in the robust summaries that accompany the Olefins Panel Resin Oils and Cyclodiene Dimer Concentrates test plan. The available health effects information indicates that DCPD is moderately toxic by relevant routes of exposure. Acute lethal oral doses in animal species are variable ranging from 0.19 g/kg in the mouse to approximately 1.2 g/kg in cattle. Lethal vapor concentrations are also variable, ranging, for 4-hour exposures, from 145 ppm for the mouse, to approximately 770 ppm for the guinea pig and rabbit. Substantially saturated vapor concentrations (2500 ppm) are lethal to rats in 60 minutes (Gage, 1970). However, the 4-hour rat LC_{50} is about 660 ppm; three of four rats survived ten 6-hour daily exposures at 250 ppm, and all survived 15 such exposures at 100 ppm. (Gage, 1970) Dogs, guinea pigs, and rabbits were more resistant than mice. (Kinkead, *et al.*, 1971) All species followed a general pattern of eye irritation, loss of a considerable degree of coordination, and if death ensued, convulsions. (Kinkead, *et al.*, 1971; ECETOC, 1991; Gage, 1970). Similar to other hydrocarbons, the predominant acute systemic effect is on the central nervous system; DCPD produces initial stimulation followed by prolonged depression. DCPD has a disagreeable odor similar to camphor and has reportedly resulted in headaches in workers following prolonged exposure to low vapor concentrations. DCPD is also irritating when directly applied to the skin and eyes and may be an aspiration hazard.

Several studies have evaluated DCPD for repeated exposure effects. The most consistent effect at non-lethal doses was to the kidneys of male rats but some studies also found effects to the lung, liver, gastrointestinal tract, and adrenal gland. In feeding studies, DCPD given for up to 90 days to mice and rats did not result in treatment-related effects at nominal dietary concentrations up to 273 ppm or 750 ppm, respectively. Dogs in a similar study exhibited some evidence of gastro-intestinal disturbance at the highest dietary concentration (1,000 ppm nominal). In the most recent study conducted by gavage and according to OECD Guideline 422 , daily exposure to 4, 20, or 100 mg/kg DCPD produced a variety of effects to male and female rats (JETOC, 1998). Two females (of ten) in that received 100 mg/kg died during treatment and (all) males and surviving females exhibited slight suppression of body weight gain and decreased feed consumption. Male rats of the high dose group demonstrated increase in liver enzymes, increased liver and kidney weight, and microscopic findings of single cell necrosis in the liver and hyaline droplets and renal tubular changes in the kidney. The kidney microscopic changes were also observed in the male rats that received 4 and 20 mg/kg DCPD. Both males and females in the 100 mg/kg group and males in the 20 mg/kg group also exhibited increase in fatty droplets in the adrenal glands. The no observed effect level doses for repeat dose toxicity for this study were considered to be 20 mg/kg/day for females and less than 4 mg/kg/day for males.

Repeated inhalation exposure of laboratory animals to DCPD vapor also produced kidney lesions in male rats of several studies. The kidney lesions described in these studies give the

appearance of the male rat specific disease hyaline droplet nephropathy, a condition not considered relevant to humans. Lung lesions described as chronic pneumonia and bronchiectasis was reported in rats exposed to 35 and 74 ppm (Kinkead *et al*., 1971); however in a second study (Bevan *et al*., 1992), no lung lesions were observed in rats repeatedly exposed to 50 ppm DCPD.

DCPD is not selectively toxic to rodent reproduction or the developing embryo/fetus. In a reproductive/developmental toxicity screening study conducted by oral gavage (JETOC, 1998), no effects were noted on reproductive parameters at up to 100 mg/kg. This dose, however, was lethal to 2 (of 10) female rats and 2 rats of this group (presumably the same animals) lost 100% of their litters during lactation (days 1-4). A low viability index and tendency to lower birth weight and body weight gain were observed in neonates in the highest dose group. The no observed effect level doses for this study were 100 mg/kg/day for parental males and 20 mg/kg/day for parental females and offspring. The NTP evaluated the potential reproductive toxicity of orally (gavage) administered DCPD (10, 30, or 100 mg/kg) in rats using a continuous breeding protocol (Jamieson *et al*., 1995). DCPD at 100 mg/kg produced lower pup weights, increased pup mortality, fewer pups born alive, and increased cumulative days to litter. In the 30 mg/kg group, only a slight (4%) reduction in the average female pup weight was observed. There were no reproductive effects observed in the 10 mg/kg group. Epididymal sperm density, percent motility, percent abnormal sperm, spermatids per milligram of testis, and total spermatids per testis were not affected by the administration of DCPD at dose levels employed in this study. There was decreased F2 pup weight in the 100 mg/kg group of the second generation. At the doses that yielded reproductive effects, parental animals exhibited effects on liver and kidney; hence the DCPD reproductive effects that were observed in this study were not considered by NTP to be selective. A 3-generation reproduction study of DCPD administered to rats in the diet at 80 and 750 ppm resulted in no deleterious effects on reproductive processes or general condition of the rats and no evidence of dose-related teratologic effect over three successive generations with two matings per generation (Hart, 1980).

Developmental toxicity range-finding studies were conducted by NTP in New Zealand White rabbits and Sprague-Dawley rats (Gulati *et al*., 1993a,b). DCPD administered by gavage at 25, 100, 200, 300, or 400 mg/kg to rabbits caused maternal toxicity at 200 mg/kg and higher doses. Gross deformities were evident at 400 mg/kg but no other developmental endpoints were significantly affected. Rats were administered DCPD at 50, 200, 300, 400, and 500 mg/kg by gavage. Body weights were significantly decreased at two time points and for body weight gain throughout the treatment for rats in the 50 and 200 mg/kg groups. Clear maternal toxicity, including maternal death, was observed at 200 mg/kg and higher doses (3/7 in the 200 mg/kg group, 8/9 in the 300 mg/kg group, and all in the 400 and 500 mg/kg groups were found dead by gestation day 9). Developmental toxicity in the form of decreased fetal weight was observed in the 200 mg/kg group. In a rat teratology study there were no effects on pregnant dams from dietary administration of 80, 250, or 750 ppm DCPD and no compound-induced terata, variation in sex ratio, embryo toxicity or inhibition of fetal growth and development (Hart, 1980). DCPD is not toxic to genetic mechanisms either in bacterial or mammalian systems. Tests for mutations and chromosomal effects have been negative for DCPD. DCPD has not been evaluated for carcinogenic effects.

Other Components

The biological activity of DCPD is expected to be similar to that of other physicochemically similar C8 to C12 cycloalkenes. There is less information available, however, for other mono- and dicyclic alkenes and their substituted derivatives as these substances are of lesser commercial interest. The toxicology properties of cycloalkenes is reviewed by Cavender (1994a). The available information for C8 to C12 cycloalkenes indicate these hydrocarbons show similar acute toxicity profiles as DCPD in terms of lethal dosages and clinical signs dominated by CNS effects. The liquid cycloalkenes in this range are also considered aspiration hazards. These hydrocarbons exhibit irritation effects with some producing severe and corrosive effects to the skin (e.g. cyclooctadiene). Some members are also skin sensitizers. There is very limited reliable information available on the toxic effects of C8 to C12 cycloalkenes following repeated exposure. A few studies have been conducted on limonene (a C10 cycloalkene that occurs in the oil of many plants). Decreases in body weight and non-specific systemic effects were noted in mice and dogs that received oral doses of limonene for up to 1 to 6 months. In male rats, limonene resulted in formation of hyaline droplets in the kidneys, a similar finding with DCPD.

The C8 to C12 aromatic hydrocarbons in general show qualitatively similar toxicological properties as the C8 to C12 cycloalkenes (Cavender, 1994a,b). There are quantitative differences, however, between these hydrocarbons with the cycloalkenes producing greater toxicity at comparable dosages. The available information for solvents that are mixtures of C8 to C12 aromatic hydrocarbons indicate in general that this range of aromatic hydrocarbons are: of low to moderate acute toxicity producing transient CNS effects at high doses, of low repeated exposure systemic toxicity, not genotoxic, and not selectively toxic to the developing fetus, embryo, or reproductive system. The specific assessment of the available toxicology information for the C8 to C12 aromatic hydrocarbons is to be included in the International Hydrocarbon Solvents Consortium C9 Aromatic Hydrocarbon Solvents and C10+ Aromatic Hydrocarbon Solvents categories and will not be discussed more specifically in this test plan.

In addition to the existing information on DCPD as the dominant and / or representative cycloalkene and on C8 to C12 aromatic hydrocarbons, there is also some limited information available on streams that consist of both kinds of hydrocarbons. As expected, the toxicological properties of the streams are not dissimilar to that of this range of cycloalkenes and aromatic hydrocarbons. Resin-Former Feedstock, a test sample that consisted of 50-60% DCPD, 15-20% cyclopentadiene/methyl cyclopentadiene dimer, < 2% butadiene dimer, 10-12% styrene, < 2% xylene, and < 2% cyclopentadiene, exhibited low acute toxicity with CNS effects presented (Rausina, 1983; Gordon, 1983a). In addition, it possesses low to moderate toxicity following repeated exposure with evidence of CNS (likely acute), liver and kidney (hydrocarbon nephropathy) effects, and generally an absence of genotoxic effects including an *in vivo* mouse micronucleus test (Rausina, 1984; Gordon, 1983b; Papciak and Goode, 1984; Brecher and Goode, 1984; Khan and Goode, 1984). This material did exhibit positive activity in one *in vitro* system, a test of cell transformation in mouse embryo cells (Brecher and Goode, 1983). Details on these studies are provided in The Resin Oils and Cyclodiene Dimer Concentrates category robust summaries.

To supplement the above data, the Olefins Panel Resin Oils and Cyclodiene Dimer Concentrates test plan proposes testing two representative streams, Low DCPD Resin Oil and DCPD/Codimer Concentrate. This testing will provide SIDS datasets for these streams which are relevant to the Fuel Oils category.

The details of the strategy are as follows:

Existing data on Fuel Oil streams and stream components, as well as new data resulting from other testing programs on components present in significant amounts in the streams of the Fuel Oils Category will be evaluated.

Stream Components will be evaluated from data from the sources indicated below:

- Dicyclopentadiene: DCPD is sponsored in the OECD SIDS program by Japan. A SIAR has been submitted.
- Naphthalene: A risk assessment is being conducted under the EU Existing Substances Directive and is expected to be completed soon.
- Biphenyl: This material has been volunteered under the HPV Challenge program by the SOCMA Biphenyl Working Group for 2003.
- Mixture of C5 olefins and aliphatic hydrocarbons: Included in the Olefins Panel C5 Non-Cyclics Category. A test plan was submitted to EPA on November 7, 2001.
- Heavy Fuel Oils (Petroleum): These chemically similar materials have been volunteered under the HPV Program by the American Petroleum Institute for 2003.
- C8 to C12 aromatic hydrocarbons: Included in the International Hydrocarbon Solvents Consortium C9 Aromatic Hydrocarbon Solvents and C10+ Aromatic Hydrocarbon Solvents categories to be addressed in OECD SIDS (ICCA). Test plans are being submitted to EPA in 2001 and 2002.
- C7 to C10 aliphatic hydrocarbons: Included in the International Hydrocarbon Solvents Consortium C7 to C9 Aliphatic Hydrocarbon Solvents and C9 to C13 Aliphatic Hydrocarbon Solvents categories to be addressed in OECD SIDS (ICCA). Test plans are being submitted to EPA in 2001 and 2002.
- The DCPD stream studies for the Olefins Panel Resin Oils and Cyclodiene Dimer Concentrates Category are described above. The test plan for this category will be submitted in 2001.

Fuel Oils Streams

Toxicology data for oral, dermal, and inhalation routes of exposure are available for the following mixed process streams that represent typical Fuel Oils. Robust summaries of relevant studies have been prepared for the following:

- Light Pyrolysis Fuel Oil

- Aromatic Pyrolysis Oil, Rerun Tower Bottoms
- Biphenyl Feedstock
- Coal Derived Fuel Oils

Existing studies of these Fuel Oils steams are indicated in Table 4, along with supporting data from studies on related materials, including two coal derived experimental fuel oils with similar composition. Mutagenicity studies, including *in vivo* mouse micronucleus assays for these streams, indicate the potential to produce point mutations, unscheduled DNA synthesis, and cell transformations, especially for heavy fuel oils. Repeated dose studies of up to lifetime duration (i.e., 28 months) indicate the potential for development of skin tumors (dermal exposure) and decreased body weight and hematological effects (dermal and inhalation exposures). Histopathological changes were observed in kidneys, adrenal glands, liver, lung, thymus and bone marrow. Results from the limited number of reproductive studies on these and related materials indicate little effect on reproductive capacity or performance; however, there were increases in specific malformations observed in developmental toxicity studies of related materials. The observed effects are likely attributable to the polycyclic aromatic hydrocarbon content that can range upward of 5%. Taken as a whole, these data suggest that the most sensitive health effects for Fuel Oils are due to the C10-12 components and polycyclic aromatic hydrocarbon content. The mammalian health hazards of these materials have been adequately characterized and no further testing will be conducted.

B. Environmental / Aquatic Effects and Test Plan Strategy

PHYSICOCHEMICAL PROPERTIES

The physicochemical (PC) endpoints for the HPV Chemical Program include:

- Melting Point
- Boiling Point
- Vapor Pressure
- Water Solubility
- Octanol/Water Partition Coefficient (K_{ow})

Although some of these data for products in the Fuel Oils Category exist, not all of these endpoints are defined, and a comprehensive and consensus database for chemicals that represent product streams in this category does not exist. Therefore, calculated PC data for selected chemical components in this category will be developed using a computer model to provide a consistent, representative data set. Also, existing measured data will be identified and provided where readily available. In addition, selected PC data will be developed for two products: one representative of a lighter product containing a larger proportion of lower molecular weight chemical, and the other representative of a heavier product.

Calculated PC data for selected chemical components in the Fuel Oils Category will be developed using the EPIWIN© computer model (EPIWIN, 1999), as discussed in the U.S. EPA document entitled *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program* (US EPA, 1999a). The use of computer

modeling for the development of these data is justified since components of the streams in this category are chemically related and expected to exhibit relatively similar environmental properties. In addition, for all the chemicals selected to represent products in this category, a calculated dataset provides a common method for the development of these values.

Boiling point, melting point, and vapor pressure ranges will be determined using the MPBPVP subroutine in EPIWIN. K_{ow} and water solubility will be calculated using KOWIN and WSKOW subroutines, respectively. There is more information on calculating data for the HPV chemical program in the EPA document titled, *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program*.

Because the HPV substances covered under the Fuel Oils Category testing plan are mixtures containing differing compositions, it is not possible to develop or calculate a single numerical value for each of the physicochemical properties. For example, a product that is a mixture of chemicals does not have a melting point, but rather a melting range. Calculated values for PC properties will be represented as a range of values according to the product's component composition.

Robust summaries characterizing the PC endpoints will be prepared upon completion of the proposed testing, and will include the calculated data and testing results.

ENVIRONMENTAL FATE

Environmental fate endpoints for the HPV Chemical Program include:

- Biodegradation
- Photodegradation
- Hydrolysis
- Fugacity

There are no data available on the biodegradability of products from this category. However, there are data for pure chemicals and complex products containing several chemicals not in this category, but which can be found in products from this category. These data can be used to initially assess the biodegradability of products in this category. The data suggest that fuel oil products have the potential to biodegrade to a significant extent. To confirm and characterize the potential of products in this category to biodegrade, two products will be tested.

Data and/or information in the form of a technical discussion will be provided for photodegradation. Chemicals in this category are not subject to hydrolysis at measurable rates, therefore information for this endpoint will be summarized in a technical review document.

Equilibrium models are used to calculate chemical fugacity, which can provide information on where a chemical is likely to partition in the environment. These data are useful in identifying environmental compartments that could potentially receive a released chemical. Fugacity data can only be calculated for individual chemicals. For the HPV Program,

environmental partitioning data will be calculated for selected chemical components of the products in this category.

A preliminary evaluation of chemicals in the Fuel Oils Category suggests that they will partition largely to the air and soil, and therefore their fate in these compartments is of environmental interest. Because the air phase may be a compartment that could potentially receive many of the chemical components in this category, data characterizing their potential for physical degradation in the atmosphere will be developed (this is discussed below under photodegradation).

1. Biodegradation

A biodegradation study was identified for a product in the Fuel Oils Category. Although there are only limited data, several studies were identified for component chemicals found in fuel oil products and for products not in this category. The product data are for complex substances that contain several hydrocarbons, some or all of which are found in this category. Results from these studies can be used as read across data to support an initial assessment of the persistence of fuel oil products in the environment. Although these data alone may not characterize the potential biodegradability of the chemically complex products in this category, they do provide an initial understanding of the fate of these products. The data suggest that products in this category have the potential to biodegrade to a significant extent.

A biphenyl feedstock (reported as CAS# 68989-41-3), a fuel oil product, exhibited 57% biodegradation after 28 days using an OECD (Organization for Economic Co-ordination and Development) 301 D, closed bottle test guideline. The chemical component biodegradation data are for benzene and two isomers of xylene, while the complex product data are for a primarily C8 alkene product, a primarily C9 alkylbenzene product, and a primarily naphthalene/alkylnaphthalene product. The pure chemicals exhibited 63 to 88% biodegradation after 28 days using an OECD 301 F, manometric respirometry test guideline. The data for the chemically complex products ranged from 29 to 78% for the same duration, using the same test procedure.

The manometric respirometry test (OECD guideline 301F) uses a continuously-stirred, closed test system, which is recommended when assessing the biodegradability of volatile materials like those in this category. This test is also recommended when evaluating complex products containing several chemical species, some of which may be minimally water-soluble.

To address the potential biodegradability of products in this category, the Panel proposed to test two products via manometric respirometry (OECD Guideline 301F). One product will be representative of a lighter product containing a larger proportion of lower molecular weight components and the second representative of a heavier product containing a larger proportion of higher molecular weight components. The data from the proposed testing will be compared to the data discussed above to determine whether products in this category are as readily biodegraded as suggested by those data.

2. Photodegradation – Photolysis

Direct photochemical degradation occurs through the absorbance of solar radiation by a chemical substance. If the absorbed energy is high enough, then the resultant excited state of the chemical may lead to its transformation. Simple chemical structures can be examined to determine whether a chemical has the potential for direct photolysis in water. First order reaction rates can be calculated for some chemicals that have a potential for direct photolysis using the procedures of Zepp and Cline (1977).

To develop information or data that will characterize the potential of products in this category to undergo direct photochemical degradation, the existing product chemical composition data and composition data that will be developed for the two products identified for biodegradation testing will be evaluated together to select a subset of chemicals that adequately represents products in this category. The selection process will consider chemical carbon number range, hydrocarbon type, and chemical structure. The UV light absorption of the selected chemicals will then be evaluated to identify those chemicals with a potential to degrade in solution. When possible, first order reaction rates will be calculated for those chemicals identified to have a potential for direct photolysis in water. The results of the calculations will be summarized in a technical discussion for this endpoint. If instead, a low potential for direct photolysis is suggested by the evaluation, a technical discussion will be prepared to summarize the findings.

3. Photodegradation – Atmospheric Oxidation

Photodegradation can be measured, EPA identifies OECD test guideline 113 as a test method (EPA, 1999b)' or estimated using models accepted by the EPA (EPA, 1999a). An estimation method accepted by the EPA includes the calculation of atmospheric oxidation potential (AOP). Atmospheric oxidation as a result of hydroxyl radical attack is not direct photochemical degradation, but rather indirect photodegradation. AOPs can be calculated using a computer model. Hydrocarbons, such as those in the Fuel Oils Category, have the potential to volatilize to air where they can react with hydroxyl radicals (OH-).

The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPIWIN, 1999) is used by OPPTS (Office of Pollution Prevention and Toxic Substances). This program calculates a chemical half-life based on an overall OH- reaction rate constant, a 12-hr day, and a given OH- concentration. This calculation will be performed for representative chemical components of products in the Fuel Oils Category. The existing product chemical composition data and composition data that will be developed for the two products identified for biodegradation testing will be evaluated together to select a subset of chemicals that adequately represents products in this category. The selection process will consider chemical carbon number range, hydrocarbon type, and chemical structure. The resulting calculations will be summarized in a robust summary for this endpoint.

4. Hydrolysis

Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond. Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985).

Chemical stability in water can be measured (EPA identifies OECD test guideline 111 as a test method) or estimated using models accepted by the EPA (EPA, 1999a). An estimation method accepted by the EPA includes a model that can calculate hydrolysis rate constants for esters, carbamates, epoxides, halomethanes, and selected alkylhalides. The computer program HYDROWIN (aqueous hydrolysis rate program for Microsoft windows) (EPIWIN, 1999) is used for this purpose by OPPTS. However, all of the chemical structures included in the Fuel Oils Category are hydrocarbons. That is, they consist entirely of carbon and hydrogen. As such they are not expected to hydrolyze at a measurable rate.

A technical document will be prepared that discusses the potential hydrolysis rates of chemicals in this category, the nature of the chemical bonds present, and the potential reactivity of this class of chemicals with water.

5. Fugacity Modeling

Fugacity based multimedia modeling can provide basic information on the relative distribution of chemicals between selected environmental compartments (i.e., air, soil, sediment, suspended sediment, water, biota). The U.S. EPA has acknowledged that computer modeling techniques are an appropriate approach to estimating chemical partitioning (fugacity is a calculated endpoint and is not measured). A widely used fugacity model is the EQC (Equilibrium Criterion) model (MacKay *et al.*, 1996). The U.S. EPA cites the use of this model in its document titled *Determining the Adequacy of Existing Data* (EPA, 1999b), which was prepared as guidance for the HPV Program.

In its document, the U.S. EPA states that it accepts Level I fugacity data as an estimate of chemical distribution values. The input data required to run a Level I model include basic physicochemical parameters; distribution is calculated as percent of chemical partitioned to 6 compartments described above within a defined unit world. Level I data are basic partitioning data that allow for comparisons between chemicals and indicate the compartment(s) to which a chemical is likely to partition.

The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, melting point, vapor pressure, and water solubility to calculate distribution within a unit world. This model will be used to calculate distribution values for representative chemical components in products from this category. Existing product chemical composition data and composition data that will be developed for the two products identified for biodegradation testing will be evaluated together to select a subset of chemicals that adequately represents products in this category. The selection process will consider chemical carbon number range, hydrocarbon type, and chemical structure. A

computer model, EPIWIN version 3.04 (EPIWIN, 1999), will be used to calculate the physicochemical properties needed to run the Level I EQC model. The resulting calculations will be summarized in a robust summary for this endpoint.

AQUATIC TOXICITY

Aquatic toxicity endpoints for the HPV Chemical Program include:

- Acute Toxicity to a Freshwater Fish
- Acute Toxicity to a Freshwater Invertebrate
- Toxicity to a Freshwater Alga

An acute invertebrate toxicity study is available on a product from this category. There are no fish or alga toxicity data available for products in this category. However, there are read across data to initially characterize these two endpoints for chemicals found in products from this category and complex products that contain chemicals found in products from this category. The data suggest that products in this category have the potential to exhibit a moderate range of toxicity for the three aquatic toxicity endpoints. The use of data from selected read across materials to products in this category can be justified for the following reasons:

- Individual chemicals and complex products used for read across purposes contain a chemical class (i.e., aromatics) that is found in products from this category.
- Individual chemicals and complex products used for read across purposes have a carbon number or carbon number range that falls within the range of carbon numbers found in products from this category.
- Individual chemicals and complex products used for read across purposes as well as a product in this category are composed of chemicals that all act by a similar mode of toxic action.

The aquatic toxicity of products in the Fuel Oil Category are expected to fall within a narrow range regardless of the varying carbon number range and constituent composition of those products. This is expected because the constituent chemicals of those products are neutral organic hydrocarbons whose toxic mode of action is non-polar narcosis. The mechanism of short-term toxicity for these chemicals is disruption of biological membrane function (Van Wezel and Opperhuizen, 1995), and the differences between toxicities (i.e., LC/LL_{50}, EC/EL_{50}) can be explained by the differences between the target tissue-partitioning behavior of the individual chemicals (Verbruggen *et al*., 2000).

The existing fish toxicity database for hydrophobic neutral chemicals supports a critical body residue (CBR, the internal concentration that causes mortality) of between approximately 2-8 mmol/kg fish (wet weight) (McCarty and MacKay, 1993; McCarty *et al*., 1991). When normalized to lipid content the CBR is approximately 50 umol/g of lipid for most organisms (Di Toro *et al*., 2000). Because most of the products in this category are composed of complex combinations of relatively similar series of homologous chemicals, their short-term toxicities are expected to fall within the range of toxicity demonstrated by the chemicals and products summarized in this test plan. Therefore, these existing data that are believed to form

a sufficiently robust dataset to initially characterize the expected range of aquatic toxicity for products in this category.

An acute invertebrate study is available for a biphenyl feedstock product (reported as CAS# 68989-41-3), a fuel oil product, in this category. The 48-hour LL50 value for *Daphnia magna* is reported as 23.6 mg/L. Because the product tested was a complex hydrocarbon material containing several chemical components, exposure solutions for each treatment level were developed as water accommodated fractions and the results reported as lethal loading (LL) values, which is the procedure recommended by OECD for these types of materials (OECD, 1999).

Table 6 lists the chemical and product data that do not belong to this category, but are being used to support the initial characterization of the aquatic toxicity of this category. The acute toxicity data are for fish and an invertebrate, and fall within an effect range of 1.1 to 23.6 mg/L.

To address whether the expected toxicity for the three aquatic endpoints falls within the range of data presented above for with this category, the Panel proposes to test two products. One product will be representative of a lighter product containing a larger proportion of lower molecular weight components and the second will be representative of a heavier product containing a larger proportion of higher molecular weight components. Acute fish, acute invertebrate, and alga toxicity tests will be conducted for each product. In addition, the chemical composition of the products tested will be characterized to the degree that predominant chemical constituents and/or carbon number and chemical class (i.e., olefin, paraffin, aromatic) will be identified.

IV. TEST PLAN SUMMARY

The existing Fuel Oils stream data, existing components data, and data under development by the American Chemistry Council for other categories under the HPV program, by other HPV consortia, and by the OECD SIDS program, will be sufficient to characterize the human health endpoints of the range of products in this category in satisfaction of HPV program requirements. Environmental fate and effects endpoints will be thoroughly characterized and a comprehensive and consensus physicochemical database for products in this category will be developed.

Aquatic testing, modeling, technical discussions, and physicochemical data will be developed for the Fuel Oils Category as described below, and as detailed in Table 5.

- Conduct acute aquatic toxicity studies on two streams representative of the light and heavy ends of the fuel oils product spectrum.
- Conduct biodegradation studies on a product from each of the same two streams.
- Prepare a technical discussion on the potential of chemical components comprising streams in this category to photodegrade.

- Prepare a technical discussion on the potential of chemical components comprising streams in this category to hydrolyze.
- Calculate fugacity data for selected chemical components of streams in this category.
- Calculate physiochemical data as described in the EPA document titled *The Use of Structure-Activity Relationships (SAR) in the High Production Volume Chemicals Challenge Program* and identify readily available data. Develop relevant measured physicochemical data for the two products selected for environmental fate and effects testing cited above.

Summaries of the results will be developed once the data and analyses are available. This test plan is expected to provide data sufficient to characterize the human health effects and environmental fate and effects endpoints for the Fuel Oils Category under the program.

V. OTHER SUPPORTING DATA

Additional data for components of the Fuel Oils streams that will provide support for this category will be collected by other test plans within the HPV program (see Table 7), by other consortia participating in the HPV or ICCA programs, or from chemicals sponsored in the OECD SIDS program. These include:

- Dicyclopentadiene: DCPD is sponsored in the OECD SIDS program by Japan. A SIAR has been submitted.
- Naphthalene: A risk assessment is being conducted under the EU Existing Substances Directive and is expected to be completed soon.
- Biphenyl: This material has been volunteered under the HPV Challenge program by the SOCMA Biphenyl Working Group for 2003.
- Heavy Fuel Oils (Petroleum): These chemically similar materials have been volunteered under the HPV Program by the American Petroleum Institute for 2003.
- C8 to C12 aromatic hydrocarbons: Included in the International Hydrocarbon Solvents Consortium C9 Aromatic Hydrocarbon Solvents and C10+ Aromatic Hydrocarbon Solvents categories to be addressed in OECD SIDS (ICCA). Test plans are being submitted to EPA in 2001 and 2002.
- C7 to C10 aliphatic hydrocarbons: Included in the International Hydrocarbon Solvents Consortium C7 to C9 Aliphatic Hydrocarbon Solvents and C9 to C13 Aliphatic Hydrocarbon Solvents categories to be addressed in OECD SIDS (ICCA). Test plans are being submitted to EPA in 2001 and 2002.
- The DCPD stream studies for the Olefins Panel Resin Oils and Cyclodiene Dimer Concentrates Category are described above. The test plan for this category will be submitted in 2001.

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Table 1. CAS Numbers used in the Fuel Oils Category

CAS #	CAS Inventory Name
64741-62-4	Clarified oils, petroleum, catalytic cracked
64742-90-1	Residues, petroleum, steam-cracked
68131-05-5	Hydrocarbon oils, process blends
68409-73-4	Aromatic hydrocarbons, biphenyl-rich
68475-80-9	Distillates, petroleum, light steam-cracked naphtha
68513-69-9	Residues, petroleum, steam-cracked light
68514-34-1	Hydrocarbons, C9-14, ethylene-manuf.-by-product
68527-18-4	Gas oils, petroleum, steam-cracked
68921-67-5	Hydrocarbons, ethylene-manuf.-by-product distn. residues
69013-21-4	Fuel oil, pyrolysis
69430-33-7	Hydrocarbons, C6-30
8002-05-9	Petroleum

Table 2. Steams Included in the Fuel Oils Category

Olefins Industry Stream
Heavy Pyrolysis Fuel Oil from the Ethylene Process Unit
Light Pyrolysis Fuel Oil from the Ethylene Process Unit
Quench Oil from the Ethylene Process Unit water quench system
Pyrolysis Fuel Oil from Pyrolysis Gasoline Distillation
Combined Fuel Oil from the Ethylene & Pyrolysis Gasoline
Combined Fuel Oil from Benzene HDA and Pyrolysis Fuel Oils
Hydrotreated Flux Oil
Biphenyl Concentrate

Table 3. Typical Stream Compositions for Fuel Oils Category

Component (See note 1, 2 and 3 at the bottom of this table.)	Heavy Pyrolysis Fuel Oil from the Ethylene Process Unit*	Quench Oil from the Ethylene Process Unit water quench system	Pyrolysis Fuel Oil from Pyrolysis Gasoline	Combined Fuel Oil from Ethylene & Pyrolysis Gasoline	Light Pyrolysis Fuel Oil from the Ethylene Process Unit	Hydro-treated Flux Oill	Biphenyl Concen-trate	Combined Fuel Oil from Benzene HDA & Pyrolysis Fuel Oils
Composition, wt %								
1,3-Butadiene		0.1 - 0.3						
C6 Non-aromatics				0.2 - 3.1				
C5s and Lighter				1.8				
C6 and Lighter								0.2
Benzene		0.1		0.2 – 4				0. 1 - 0.3
C7 Paraffins & Napththenes				3				
Toluene		5		0.2 – 1.3			1 - 8	
C8 Paraffins & Naphthenes				6.1				
Ethylbenzene		5					1	
C8 Aromatics				0.4 – 2.6				
Xylenes, Mixed		5					2	
Styrene		0 - 5		0.9				
C9 Aromatics			2	12.6				
Other Benzenes to Naphthalene				14.5				11
C9 Paraffins & Naphthenes				12.6				
C10+ (NOS)							20 – 25	
Trimethylbenzenes				1				
Dicyclopentadiene			20	0.9				7.5 - 11.7
C10 & C11 Codimers of C5&C6			30					
Indane (Indan)				1.5				
2,3-Benzindene				2 – 5				5 - 6.4
Methyl Dicyclopentadiene				0.9				
C10 Aromatics				32.1		7.6		
C11 Isoparaffins						26.7		
1,4-Dimethyl-2-ethylbenzene						1.9		
1,4-Methyl-t-butylbenzene						2.8		
Undecene-1						0.8		
Indene		5	2	0.7 - 0.8	5 – 15			3.8
1,2,3,5-Tetramethylbenzene (Isodurene)						2.4		
Methyl Indenes				5.6				0.2 – 2
C12 Isoparaffins						5.9		
4-Methylindan						2.3		
2-Methylindan						4.4		
1,3-Methyl-n-butylbenzene						5.4		
1,3-Di-i-propylbenzene						7.8		
1,3-Diethyl-5-methylbenene				1.5				
Dimethyindan				4.0				
Dimethylindene				5.4				

Component (See note 1, 2 and 3 at the bottom of this table.)	Heavy Pyrolysis Fuel Oil from the Ethylene Process Unit*	Quench Oil from the Ethylene Process Unit water quench system	Pyrolysis Fuel Oil from Pyrolysis Gasoline	Combined Fuel Oil from Ethylene & Pyrolysis Gasoline	Light Pyrolysis Fuel Oil from the Ethylene Process Unit	Hydro-treated Flux Oill	Biphenyl Concen-trate	Combined Fuel Oil from Benzene HDA & Pyrolysis Fuel Oils
Composition, wt %								
n-C13				1.3				
Methylcyclopentadiene Dimers				5.1				
C11 Aromatics						4.6		
Naphthalene	0 - 4	0.7 - 10	7	10 - 47	30 - 60	7.3	1 - 4	7 - 13.2
1,3,5-Triethylbenzene						2.4		
C12 Aromatics						3.5		
Dodecene-1						0.7		
C13 Isoparaffins						0.6		
C7-C18 Cyclic Olefins		65.0						
Methylnaphthalene				3.8 - 30			1	
2-Methylnaphthalene			2					0.1 – 13
1-Methylnaphthalene			2					9
Fluoranthene		0 - 1.1						
1,1'-Biphenyl		0.5 - 5	6	1.1 - 5.1			65 - 95	25 - 34.6
Ethyl Naphthalene's				0.8				1.5 - 4
Substituted Napthalenes			13					
1-Ethylnaphthalene			8					
Dimethylnapthalenes			8	3.8				
Acenaphthylene		0.1 - 6.9						
Diphenylethane				2 – 7				
Acenaphthene		0.1 - 1.3						2
Fluorene				3				
C10 Parafins & Naphthenes				1.1				
C14+						2.5		
Phenanthrene				5				7
Anthracene		10		1 - 5				2
Heavy Hydrocarbons and Polycyclic Aromatics			7.0					
Terphenyls								2.5
Methylbiphenyls				5 - 10			1 - 3	6.2
>C18 Cyclic Olefins		5						
1,2-Dihydroacenaphthylene			1					

NOS not otherwise specified
* Consists of C10+ and polycyclic aromatic hydrocarbons, NOS.
Note 1: The composition data shown are composites of reported values.
Note 2: The balance of these streams is expected to be other hydrocarbons that have boiling points in the range of the listed components.
Note 3: The listed highs and lows should not be considered absolute values for these limits. They are instead the highs and lows of the reported values.

Table 4. Existing Data To Use for Evaluation of Streams in Fuel Oils Category

Robust summaries for available data submitted separately.

	Human Health Effects						Environmental Toxicity			Physical Chem.	Environmental Fate			
Stream Description/Stream Component	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Repeated Dose	Develop-mental	Reproduc-tion	Acute Fish	Acute Inverte-Brate	Algal Toxicity		Photo-deg.	Hydro-lysis	Fugacity	Biodeg-radation
Biphenyl feedstock	√	√	√					√						√
Aromatic pyrolysis oil	√	√	√											
Rerun tower bottoms	√	√	√	√	√									
Light pyrolysis fuel oil	√	√	√	√										
Pyrolysis fuel oil				√										
EDS experimental fuel oils (ETP 19 and 70/30)	√	√		√	√	√								
Heavy coker gas oil	√	√	√	√	√									

Table 5. Assessment Plan for Streams in Fuel Oils Category Under the Program.

	Human Health Effects						Environmental Toxicity			Physical Chem.	Environmental Fate			
Stream Description/Stream Component	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Repeated Dose	Develop-mental	Reproduc-tion	Acute Fish	Acute Inverte-Brate	Algal Toxicity		Photo-deg.	Hydro-lysis	Fugacity	Biodeg-radation
Light fuel oil (typical)	RA	RA	RA	RA	RA	RA	T	T	T	T/SAR	TD	TD	CM	T
Heavy fuel oil (typical)	RA	RA	RA	RA	RA	RA	T	T	T	T/SAR	TD	TD	CM	T

A Adequate existing data available
CM Computer modeling proposed
NA Not applicable
TD Technical discussion proposed
T Testing proposed
RA Read-Across to existing data (see table 4)
SAR Structure-Activity-Relationship modeling and readily available data

Table 6. Aquatic Toxicity Data by Endpoint and Carbon Number(s) for a Fuel Oil Product, and Chemicals and Chemically Complex Products with Chemical Constituents that can be Found in Fuel Oils Category Products

TEST ORGANISM & ENDPOINT	CHEMICAL OR COMPLEX PRODUCT BY CARBON NUMBER(S)*[1]							
	C8 o-X[2]	**C8 m-X**[2]	**C8 p-X**[2]	**C9 EB**[3]	**C9 AB**[4]	**C10 N**[5]	**C10/12 N/AN**[6]	**C10/12 BP**[7]
Fish 96-hr LC_{50} (mg/L)	16.4 Fm	-	2.6 Rt	12.1 Fm	-	-	-	-
Daphnid EC_{50} (mg/L)	1.0 *Dm* [a]	4.7 *Dm* [a]	-	-	-	16.7 *Dm* [b]	-	-
Fish 96-hr LL_{50} (mg/L)	-	- -	- -	- -	18.0 Rt	-	3.0 Rt	-
Daphnid 48-hr EL_{50} (mg/L)	-	-	-	-	21.3 *Dm*	-	1.1 *Dm*	23.6 *Dm*

* Robust summaries for all materials except the biphenyl feedstock product (BP) are from the International Hydrocarbon Solvents Consortium and will be contained in selected SIARs (to be submitted)
1 Predominant carbon number(s) for complex products
2 Xylene (chemical)
3 Ethylbenzene (chemical)
4 Alkylbenzenes (complex product, predominantly C9)
5 Naphthalene (chemical)
6 Naphthalene / Alkylnaphthalenes (complex product, predominantly C10/11)
7 Biphenyl Feedstock (complex fuel oil product, predominantly C10-12 hydrocarbons)

LC/EC Lethal/Effect concentration
LL / EL Lethal / Effect loading
Fm Fathead minnow
Rt Rainbow trout
Dm[a] *Daphnia magna* - 24 hr study
Dm[b] Daphnia magna - 48 hr study

Table 7. Olefins Panel Sponsored HPV Test Categories

Category Number	Category Description
1	Crude 1,3-Butadiene C4
2	Low 1,3-Butadiene C4
3	C5 Non-Cyclics
4	Propylene Streams (3) – Propylene sponsored through ICCA
5	High Benzene Naphthas
6	Low Benzene Naphthas
7, 8, 9	Resin Oils and Cyclodiene Dimer Concentrates
10	Fuel Oils

Appendix I

ETHYLENE PROCESS DESCRIPTION

A. The Ethylene Process

1. Steam Cracking

Steam cracking is the predominant process used to produce ethylene. Various hydrocarbon feedstocks are used in the production of ethylene by steam cracking, including ethane, propane, butane, and liquid petroleum fractions such as condensate, naphtha, and gas oils. The feedstocks are normally saturated hydrocarbons but may contain minor amounts of unsaturated hydrocarbons. These feedstocks are charged to the coils of a cracking furnace. Heat is transferred through the metal walls of the coils to the feedstock from hot flue gas, which is generated by combustion of fuels in the furnace firebox. The outlet of the cracking coil is usually maintained at relatively low pressure in order to obtain good yields to the desired products. Steam is also added to the coil and serves as a diluent to improve yields and to control coke formation. This step of the ethylene process is commonly referred to as "steam cracking" or simply "cracking" and the furnaces are frequently referred to as "crackers".

Subjecting the feedstocks to high temperatures in this manner results in the partial conversion of the feedstock to olefins. In the simplest example, feedstock ethane is partially converted to ethylene and hydrogen. Similarly, propane, butane, or the hydrocarbon compounds that are associated with the liquid feedstocks are also converted to ethylene. Other valuable hydrocarbon products are also formed, including other olefins, diolefins, aromatics, paraffins, and lesser amounts of acetylenes. These other hydrocarbon products include compounds with two or more carbon atoms per molecule, i.e., C2, C3, C4, etc. Propane and propylene are examples of C3 hydrocarbons and benzene, hexene, and cyclohexane are a few examples of the C6 hydrocarbons.

2. Refinery Gas Separation

Ethylene and propylene are also produced by separation of these olefins streams, such as from the light ends product of a catalytic cracking process. This separation is similar to that used in steam crackers, and in some cases both refinery gas streams and steam cracking furnace effluents are combined and processed in a single finishing section. These refinery gas streams differ from cracked gas in that the refinery streams have a much narrower carbon number distribution, predominantly C2 and/or C3. Thus the finishing of these refinery gas streams yields primary ethylene and ethane, and/or propylene and propane.

B. Products of the Ethylene Process

The intermediate stream that exits the cracking furnaces (i.e., the furnace effluent) is forwarded to the finishing section of the ethylene plant. The furnace effluent is commonly referred to as "cracked gas" and consists of a mixture of hydrogen, methane, and various hydrocarbon compounds with two or more carbon atoms per molecule (C2+). The relative amount of each component in the cracked gas varies depending on what feedstocks are cracked and cracking process variables. Cracked gas may also contain relatively small concentrations of organic sulfur compounds that were present as impurities in the feedstock or were added to the feedstock to control coke formation. The cracked gas stream is cooled, compressed and then separated into the individual streams of the ethylene process. These streams can be sold commercially and/or put into further steps of the process to produce additional materials. In some ethylene processes, a liquid fuel oil product is produced when the cracked gas is initially cooled. The ethylene process is a closed process and the products are contained in pressure systems.

The final products of the ethylene process include hydrogen, methane (frequently used as fuel), and the high purity products ethylene and propylene. Other products of the ethylene process are typically mixed streams that are isolated by distillation according to boiling point ranges. It is a subset of these mixed streams that make up the constituents of the Fuel Oils Category. See Figure 1 for a schematic.

Figure 1
Chemical Process Operations Associated With Process Streams in the Fuel Oils Category